

Discrepancy, separation and Riesz energy of finite point sets on compact connected Riemannian manifolds

Paul Leopardi

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Abstract On a smooth compact connected d -dimensional Riemannian manifold M , if $0 < s < d$ then an asymptotically equidistributed sequence of finite subsets of M that is also well-separated yields a sequence of Riesz s -energies that converges to the energy double integral, with a rate of convergence depending on the geodesic ball discrepancy. This generalizes a known result for the sphere.

Keywords compact Riemannian manifold · ball discrepancy · equidistribution · separation · Riesz energy

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1 Introduction and Main Results

This paper arises from a remark at the end of the related paper [19] on separation, discrepancy and energy on the unit sphere, that the results of Blümlinger [3] could be used to generalize the results given there. The main result of that paper is that, for the unit sphere $\mathbb{S}^d \in \mathbb{R}^{d+1}$, with $d \geq 2$, if $0 < s < d$ then an asymptotically equidistributed sequence of spherical codes that is also well-separated yields a sequence of Riesz s -energies that converges to the energy double integral, with the rate of convergence depending on the spherical cap discrepancy [19, Theorem 1.1]. This paper generalizes that result to the setting of the volume measure on a Riemannian manifold, with a potential based on geodesic distance.

The relationships between discrepancy and energy of measures on a manifold have been studied for a long time, in various settings, and there is an extensive literature, including works by Benko, Damelin, Dragnev, Hardin, Hickernell, Ragozin, Saff, Totik, Zeng and many others [1, 9, 15, 21]. (See also the bibliography of the related work on the unit sphere [19] for further references specific to that setting.) Many of these works have concentrated on equilibrium measure [1, 9, 21] and on manifolds

embedded in Euclidean space, with a potential based on Euclidean distance [1, 15]. In contrast, this paper focuses on the volume measure on a Riemannian manifold, with a potential based on geodesic distance. As a consequence, many results from the literature, concerning, e.g. the support of an equilibrium measure [1] do not apply here. Instead, this paper takes the approach of translating the methods used in [19] to the setting of Riemannian geometry.

For $d \geq 1$ let M be a smooth connected d -dimensional Riemannian manifold, without boundary, with metric g and geodesic distance dist , such that M is compact in the metric topology of dist . Let $\text{diam}(M)$ be the *diameter* of M , the maximum geodesic distance between points of M . Let λ_M be the volume measure on M given by the volume element corresponding to the metric g . Since M is compact, it has finite diameter and finite volume. Let σ_M be the probability measure $\lambda_M / \lambda_M(M)$ on M . For the remainder of this paper, all compact connected Riemannian manifolds are assumed to be finite dimensional, smooth and without boundary, unless otherwise noted.

For any probability measure μ on M , the *normalized ball discrepancy* is

$$\mathcal{D}(\mu) := \sup_{x \in M, r > 0} |\mu(B(x, r)) - \sigma_M(B(x, r))|,$$

where $B(x, r)$ is the geodesic ball of radius r about the point x [3, 8].

This paper concerns infinite sequences $\mathcal{X} := (X_1, X_2, \dots)$ of finite subsets of the manifold M . Each such finite subset is called an *M-code*, by analogy with spherical codes, which are finite subsets of the unit sphere \mathbb{S}^d . A sequence (X_1, X_2, \dots) whose corresponding sequence of cardinalities $(|X_1|, |X_2|, \dots)$ diverges to $+\infty$ is called a *pre-admissible* sequence of *M-codes*.

An *M-code* X with cardinality $|X|$ has a corresponding probability measure σ_X and normalized ball discrepancy $\mathcal{D}(X)$, where for any measurable subset $S \subset M$,

$$\sigma_X(S) := |S \cap X| / |X|,$$

and

$$\mathcal{D}(X) := \mathcal{D}(\sigma_X) = \sup_{y \in M, r > 0} ||B(y, r) \cap X| / |X| - \sigma_M(B(y, r))|.$$

It is easy to see that $\mathcal{D}(X) \geq 1/|X|$, since for any $x \in X$, $\sigma_M(B(x, r))$ can be made arbitrarily small by taking $r \rightarrow 0$, while $\sigma_X(B(x, r))$ must always remain at least $1/|X|$, since the ball $B(x, r)$ contains the point $x \in X$.

A pre-admissible sequence $\mathcal{X} := (X_1, X_2, \dots)$, of *M-codes* with corresponding cardinalities $N_\ell := |X_\ell|$ is *asymptotically equidistributed* [8, Remark 4, p. 236], if the normalized ball discrepancy is bounded above as per

$$\mathcal{D}(X_\ell) < \delta(N_\ell), \tag{1}$$

where $\delta : \mathbb{N} \rightarrow (0, 1]$, is a positive decreasing function with $\delta(N) \rightarrow 0$ as $N \rightarrow \infty$.

By the *minimum geodesic distance* of a code X , we mean the minimum, over all pairs (x, y) of distinct code points in X , of the geodesic distance $\text{dist}(x, y)$. The pre-admissible sequences of M -codes of most interest for this paper are those such that the minimum geodesic distance is bounded below as per

$$\text{dist}(x, y) > \Delta(N_\ell) \quad \text{for all } x, y \in X_\ell, \quad (2)$$

where $\Delta : \mathbb{N} \rightarrow (0, \infty)$, is a positive decreasing function with $\Delta(N) \rightarrow 0$ as $N \rightarrow \infty$.

Flatto and Newman [12, Theorem 2.2], in the case where the manifold M is C^4 rather than smooth, showed that there exists a positive constant γ , depending on M , such that a sequence of M -codes exists with $\Delta(N_\ell) = \gamma N_\ell^{-1/d}$. In the case of smooth manifolds, as treated here, we call such a sequence of M -codes *well separated* with *separation constant* γ .

An easy area argument shows that the order $O(N^{-1/d})$ is best possible, in the sense that, for any sequence of M -codes, any applicable lower bound of the form (2) is itself bounded above by

$$\Delta(N_\ell) = O(N_\ell^{-1/d}),$$

(as $\ell \rightarrow \infty$).

For the purposes of this paper, we define an *admissible sequence* of M -codes to be a pre-admissible sequence \mathcal{X} , such that a discrepancy function δ and a separation function Δ exist, satisfying the bounds (1) and (2) respectively.

For $0 < s < d$, the *normalized Riesz s -energy* of an M -code X is $E_X U^{(s)}$, where E_X is the normalized discrete energy functional

$$E_X u := \frac{1}{|X|^2} \sum_{x \in X} \sum_{\substack{y \in X \\ y \neq x}} u(\text{dist}(x, y)),$$

for $u : (0, \infty) \rightarrow \mathbb{R}$, and $U^{(s)}(r) := r^{-s}$, the Riesz potential function, for $r \in (0, \infty)$.

The corresponding normalized continuous energy functional is given by the double integral [10, 16]

$$E_M u := \int_M \int_M u(\text{dist}(x, y)) d\sigma_M(y) d\sigma_M(x).$$

The main result of this paper is the following theorem.

Theorem 1.1 *Let M be a compact connected d -dimensional Riemannian manifold. If $0 < s < d$ then, for a well separated admissible sequence \mathcal{X} of M -codes, the normalized Riesz s -energy converges to the energy double integral of the normalized volume measure σ_M as $|X_\ell| \rightarrow \infty$. The rate of convergence of the energy difference is of order $\delta(|X_\ell|)^{(1-s/d)/(d+2-s/d)}$, where $\delta(|X_\ell|)$ is an upper bound on the geodesic ball discrepancy of X_ℓ . That is,*

$$\left| (E_{X_\ell} - E_M) U^{(s)} \right| = O\left(\delta(|X_\ell|)^{(1-s/d)/(d+2-s/d)} \right), \quad (3)$$

and therefore

$$\left| (E_{X_\ell} - E_M) U^{(s)} \right| \rightarrow 0 \quad \text{as } |X_\ell| \rightarrow \infty.$$

The proof of Theorem 1.1 is given in Section 3 below. This proof is similar to that of Theorem 1.1 in the corresponding paper on the unit sphere [19], except for two key points of difference:

1. The normalized mean potential function

$$\Phi_M^{(s)}(x) := \int_M U^{(s)}(\text{dist}(x, y)) d\sigma_M(y)$$

may vary with x , unlike the case of the sphere, where the corresponding mean potential function is a constant.

2. The volume of a geodesic ball in general does not behave in exactly the same way as the volume of a spherical cap. Luckily the appropriate estimate is good enough to obtain the result.

Blümlinger [3, Lemma 2] gives an estimate related to the Bishop-Gromov inequality [2, 11.10, pp. 253–257] [13, Lemma 5.3bis pp. 65–66] [14, Lemma 5.3bis pp. 275–277]. In the notation used here, Blümlinger’s estimate states:

Let M be a compact connected d -dimensional Riemannian manifold. Then

$$\frac{\lambda_M(B(x, r))}{\mathcal{V}_d(r)} - 1 = O(r^2)$$

(as $r \rightarrow 0$) uniformly in M , where $x \in M$ and $\mathcal{V}_d(r)$ is the volume of the Euclidean ball of radius r in \mathbb{R}^d . That is, the unnormalized volume of a small enough geodesic ball in M is similar to the volume of a ball of the same radius in \mathbb{R}^d , to the order of the square of the radius.

Remarks.

1. Blümlinger’s paper treats smooth compact connected Riemannian manifolds M whose Riemannian measure λ is such that $\lambda(M) = 1$ [3, p. 178], but it is clear from the statement of Lemma 2 and its proof that the result also applies to M where $\lambda(M)$ is any positive value.
2. Flatto and Newman [12, Theorem 2.3 and Remarks] prove a similar result, with an estimate of order $O(r)$ for C^4 manifolds, and order $O(r^2)$ for C^5 manifolds.

The proof of Lemma 2 in Blümlinger’s paper [3] makes it clear that the order estimate is valid for $r < R_0$, where R_0 is the *injectivity radius* of M [2, Lemma 3, Section 8.2, p. 153] [22, Definition 4.12, p. 110]. Thus, Blümlinger’s estimate can be restated as the following result.

Lemma 1.2 *Let M be a compact connected d -dimensional Riemannian manifold, and let R_0 be the injectivity radius of M . There exists a real positive constant C_0 such that for $r \in (0, R_0)$ and any $x \in M$,*

$$\left| \frac{\lambda_M(B(x, r))}{\mathcal{V}_d(r)} - 1 \right| \leq C_0 r^2. \quad (4)$$

2 Notation and results used in the proof of Theorem 1.1

The proof of Theorem 1.1 needs some notation and a few more results, which are stated here.

Firstly note that this paper, in common with the previous paper [19] uses “big-Oh” and “big-Omega” notation with *inequalities* in a somewhat unusual way, to avoid a proliferation of unknown constants. For upper bounds, when we say that

$$f(n) \leq g(n) + O(h(n)) \quad \text{as } n \rightarrow \infty,$$

we mean that there exist positive constants C and M such that

$$f(n) \leq g(n) + C(h(n)) \quad \text{for all } n \geq M.$$

For lower bounds, when we say that

$$f(n) \geq g(n) + \Omega(h(n)) \quad \text{as } n \rightarrow \infty,$$

we mean that there exist positive constants C and M such that

$$f(n) \geq g(n) + C(h(n)) \quad \text{for all } n \geq M.$$

Finally, when we say that

$$f(n) = g(n) + \Theta(h(n)) \quad \text{as } n \rightarrow \infty,$$

we mean that there exist positive constants $c < C$ and M such that

$$g(n) + c(h(n)) \leq f(n) \leq g(n) + C(h(n)) \quad \text{for all } n \geq M.$$

If more than one O , Ω or Θ expression is used in an inequality, the implied constants may be different from each other.

The next three results follow from Blümlinger’s estimate.

Lemma 2.1 *Let M be a compact connected d -dimensional Riemannian manifold. There is a radius $R_1 > 0$ and parameters $0 < C_L < C_H$, depending on R_1 , such that for all $x \in M$ and all $r \in (0, R_1)$,*

$$C_L r^d \leq \sigma_M(B(x, r)) \leq C_H r^d. \quad (5)$$

The ratio C_H/C_L can be made arbitrarily close to 1 by taking R_1 small enough.

Proof

Let $R_0 > 0$ be the injectivity radius of M , so that Blümlinger’s estimate (4) holds for $r \in (0, R_0)$. Note that for each d , $\mathcal{V}_d(r) = c_d r^d$, where $c_d := \mathcal{V}_d(1) > 0$. It follows that for all $r \in (0, R_0)$ the estimate

$$c_d r^d (1 - C_0 r^2) \leq \lambda_M(B(x, r)) \leq c_d r^d (1 + C_0 r^2) \quad (6)$$

holds for some $C_0 > 0$. Let $R_1 \in (0, R_0)$ satisfy $C_0 R_1^2 < 1$ so that the lower bound in the estimate (6) is positive for $r \in (0, R_1]$. It follows that for all $r \in (0, R_1)$,

$$0 < \frac{c_d(1 - C_0 R_1^2)}{\lambda_M(M)} r^d \leq \sigma_M(B(x, r)) \leq \frac{c_d(1 + C_0 R_1^2)}{\lambda_M(M)} r^d.$$

The estimate (5) therefore holds for R_1 as above, $C_L := c_d(1 - C_0 R_1^2)/\lambda_M(M)$, and $C_H := c_d(1 + C_0 R_1^2)/\lambda_M(M)$. In this case,

$$\frac{C_H}{C_L} = \frac{1 + C_0 R_1^2}{1 - C_0 R_1^2} \rightarrow 1, \quad \text{as } R_1 \rightarrow 0. \quad \square$$

Lemma 2.2 *Let M be a compact connected d -dimensional Riemannian manifold. There are positive constants $C_{bot} < C_{top}$ depending only on M , such that for all $x \in M$ and all $r \in (0, \text{diam}(M)]$,*

$$C_{bot} r^d \leq \sigma_M(B(x, r)) \leq C_{top} r^d. \quad (7)$$

Proof

Let R_1 , C_L and C_H be as in the statement of Lemma 2.1 and its proof.

For $r \in [R_1, \text{diam}(M)]$, the following inequalities hold:

$$C_L \frac{R_1^d}{\text{diam}(M)^d} r^d \leq C_L R_1^d \leq \sigma_M(B(x, R_1)) \leq \sigma_M(B(x, r)) \leq 1 \leq \frac{1}{R_1^d} r^d.$$

Thus the inequality (7) is satisfied with $C_{bot} := C_L R_1^d / \text{diam}(M)^d$ and $C_{top} := \max(C_H, R_1^{-d})$. \square

Lemma 2.3 *Let M be a compact connected d -dimensional Riemannian manifold. For $x \in M$ and real $r > t > 0$ let $n_M(x, r, t)$ be the maximum number of disjoint geodesic balls of radius t that can be contained in the ball $B(x, r)$. Then there is a constant C_2 such that for all $x \in M$, $r \in (0, \text{diam}(M))$, and $q \in (0, r)$,*

$$n_M(x, r + q/2, q/2) \leq C_2 (r/q)^d. \quad (8)$$

In other words, for real positive r , for $0 < q < r$, the maximum number of geodesic balls of radius $q/2$ that can be contained in a geodesic ball of radius $r + q/2$ is of order $O(r/q)^d$, uniformly in M .

Proof

The total volume of the small balls cannot be greater than the volume of the large ball containing them. Using Lemma 2.2, it therefore holds for $0 < q < r \leq \text{diam}(M) - q/2$ that

$$\begin{aligned} n_m(x, r + q/2, q/2) &\leq \frac{\max_{y \in M} \sigma_M(B(y, r + q/2))}{\min_{z \in M} \sigma_M(B(z, q/2))} \\ &\leq 2^d \frac{C_{top}}{C_{bot}} \left(1 + \frac{q}{2r}\right)^d (r/q)^d \leq 3^d \frac{C_{top}}{C_{bot}} (r/q)^d. \end{aligned}$$

For $r > \text{diam}(M) - q/2$, the following relationships therefore hold:

$$\begin{aligned} n_M(x, r + q/2, q/2) &= n_M(x, \text{diam}(M), q/2) \\ &\leq 3^d \frac{C_{top}}{C_{bot}} ((\text{diam}(M) - q/2)/q)^d \leq 3^d \frac{C_{top}}{C_{bot}} (r/q)^d. \end{aligned}$$

Thus (8) holds with $C_2 := 3^d C_{top}/C_{bot}$. \square

The remaining lemmas in this Section as well as the proof of Theorem 1.1 make use of the following definitions.

For $x \in M$, real radius $r > 0$, and integrable $f : B(x, r) \rightarrow \mathbb{R}$, the normalized integral of f on the geodesic ball $B(x, r)$ is

$$\mathcal{J}_{B(x, r)} f := \int_{B(x, r)} f(y) d\sigma_M(y).$$

For integrable $f : M \rightarrow \mathbb{R}$ the mean of f on M is

$$\mathcal{J}_M f := \int_M f(y) d\sigma_M(y).$$

For a function $f : M \rightarrow \mathbb{R}$ that is finite on the M -code X , the mean of f on X is

$$\mathcal{J}_X f := \int_M f(y) d\sigma_X(y) = \frac{1}{|X|} \sum_{y \in X} f(y).$$

For an M -code X , a point $x \in M$ and a measurable subset $S \subset M$, the punctured normalized counting measure of S with respect to X , excluding x is

$$\sigma_X^{[x]}(S) := |S \cap X \setminus \{x\}| / |X|,$$

and for a function $f : M \rightarrow \mathbb{R}$ that is finite on $X \setminus \{x\}$, the corresponding punctured mean is

$$\mathcal{J}_X^{[x]} f := \int_M f(y) d\sigma_X^{[x]}(y) = \frac{1}{|X|} \sum_{\substack{y \in X \\ y \neq x}} f(y).$$

Note the division by $|X|$ rather than $|X| - 1$.

The kernel $U^{(s)}(\text{dist}(x, y)) = \text{dist}(x, y)^{-s}$ is called the Riesz s -kernel. For a point $x \in M$, define the function $U_x^{(s)} : M \setminus \{x\} \rightarrow \mathbb{R}$ as

$$U_x^{(s)}(y) := U^{(s)}(\text{dist}(x, y)).$$

The mean Riesz s -potential at x with respect to M is then

$$\Phi_M^{(s)}(x) = \mathcal{J}_M U_x^{(s)}, \tag{9}$$

and the normalized energy of the Riesz s -potential on M is

$$E_M U^{(s)} = \mathcal{J}_M \Phi_M^{(s)} = \int_M \int_M \text{dist}(x, y)^{-s} d\sigma_M(y) d\sigma_M(x).$$

For an M -code X , the mean Riesz s -potential at x with respect to X but excluding x is

$$\Phi_X^{(s)}(x) := \mathcal{J}_X^{[x]} U_x^{(s)},$$

the normalized energy of the Riesz s -potential on X is

$$E_X U^{(s)} = \mathcal{J}_X \Phi_X^{(s)} = \frac{1}{|X|^2} \sum_{x \in X} \sum_{\substack{y \in X \\ y \neq x}} \text{dist}(x, y)^{-s},$$

and the mean on X of the mean Riesz s -potential is

$$\mathcal{J}_X \Phi_M^{(s)} = \frac{1}{|X|} \sum_{x \in X} \int_M \text{dist}(x, y)^{-s} d\sigma_M(y).$$

The following bound is used in Lemma 2.5 below to prove the continuity of the mean Riesz s -potential.

Lemma 2.4 *Let M be a compact connected d -dimensional Riemannian manifold. Then for the radius R_1 as per Lemma 2.1, there is a constant C_3 such that for all $x \in M$ and $r \in (0, R_1)$, the normalized integral of the function $U_x^{(s)}$ is bounded as*

$$\mathcal{J}_{B(x, r)} U_x^{(s)} \leq C_3 r^{d-s}. \quad (10)$$

Proof

Fix $x \in M$, and let $\mathcal{V}_M(r) := \sigma_M(B(x, r))$. Then for $r \in (0, R_1)$, the following equations and inequality hold,

$$\begin{aligned} \mathcal{J}_{B(x, r)} U_x^{(s)} &= \int_{B(x, r)} \text{dist}(x, y)^{-s} d\sigma_M(y) = \int_0^r t^{-s} d\mathcal{V}_M(t) \\ &= r^{-s} \mathcal{V}_M(r) + s \int_0^r t^{-s-1} \mathcal{V}_M(t) dt \\ &\leq C_H r^{d-s} + s \int_0^r C_H t^{d-s-1} dt = C_H \frac{d}{d-s} r^{d-s}, \end{aligned}$$

where the inequality is a result of Lemma 2.1. Thus the estimate (10) is satisfied for $C_3 = C_H d/(d-s)$. \square

The proof of Theorem 1.1 uses the continuity of the mean Riesz s -potential, as shown by the following lemma.

Lemma 2.5 *Let M be a compact connected d -dimensional Riemannian manifold. Then for $s \in (0, d)$, the mean Riesz s -potential $\Phi_M^{(s)}$ defined by (9) is continuous on M .*

Proof

We show that the mean Riesz s -potential $\Phi_M^{(s)}$ is continuous by using the method of proof of Kellogg [17, p. 150-151].

Let $x \in M$ and recall that $\Phi_M^{(s)}(x) = \mathcal{J}_M U_x^{(s)}$. Let x' be another point of M and consider the ball $B'_r := B(x', r)$, for some $r \in (0, R_1/3)$ where R_1 is a suitable radius as per Lemma 2.1. Consider $\Phi_{B'_r}^{(s)}(x) := \mathcal{J}_{B'_r} U_x^{(s)}$. Since $U_x^{(s)} > 0$, it is always the case that $\Phi_{B'_r}^{(s)}(x) \geq 0$. Either $\text{dist}(x, x') \leq 2r$, in which case $x' \in B(x, 2r)$ so that

$$\mathcal{J}_{B'_r} U_x^{(s)} < \mathcal{J}_{B(x, 3r)} U_x^{(s)} \leq 3^{d-s} C_3 r^{d-s}$$

as per Lemma 2.4, or $\text{dist}(x, x') > 2r$, so that

$$\mathcal{J}_{B'_r} U_x^{(s)} \leq r^{-s} C_H r^d = C_H r^{d-s},$$

as per Lemma 2.1. Therefore $\Phi_{B'_r}^{(s)} \rightarrow 0$ uniformly on M as $r \rightarrow 0$.

So, given $\varepsilon > 0$ we can take r small enough that $\Phi_{B'_r}^{(s)}(x) < \varepsilon/2$ for all $x \in M$, and therefore $\Phi_{B'_r}^{(s)}(x') < \varepsilon/2$, so

$$\left| \mathcal{J}_{B'_r} \left(U_x^{(s)} - U_{x'}^{(s)} \right) \right| < \varepsilon/2.$$

With B'_r fixed, there is a distance $t > 0$ such that when $\text{dist}(x, x') \leq t$, we have

$$\left| U_x^{(s)}(y) - U_{x'}^{(s)}(y) \right| = \left| \text{dist}(x, y)^{-s} - \text{dist}(x', y)^{-s} \right| \leq \varepsilon/2$$

for all $y \in M \setminus B'_r$. In this case

$$\left| \mathcal{J}_{M \setminus B'_r} \left(U_x^{(s)} - U_{x'}^{(s)} \right) \right| \leq \mathcal{J}_{M \setminus B'_r} \left| U_x^{(s)} - U_{x'}^{(s)} \right| < \varepsilon/2.$$

Therefore $\left| \mathcal{J}_M \left(U_x^{(s)} - U_{x'}^{(s)} \right) \right| \leq \varepsilon$ whenever $\text{dist}(x, x') \leq t$. \square

In fact, a stronger result holds, giving an estimate that is used in the proof of Theorem 1.1.

Lemma 2.6 *Let M be a compact connected d -dimensional Riemannian manifold. Then for $s \in (0, d)$, the mean Riesz s -potential $\Phi_M^{(s)}$ defined by (9) is Hölder continuous on M , with exponent $(d-s)/(d+1)$. Specifically, for $0 \leq t < \min(1, (R_1/3)^{d+1})$, the estimate*

$$\left| \Phi_M^{(s)}(x) - \Phi_M^{(s)}(x') \right| = O\left(t^{(d-s)/(d+1)}\right) \quad (11)$$

holds whenever $\text{dist}(x, x') \leq t$.

Proof

We prove (11) by putting explicit estimates into the proof of Lemma 2.5 above. This proof therefore uses the notations and the definitions used there.

Firstly, the proof of Lemma 2.5 establishes that for $r \in (0, R_1/3)$, where R_1 is a suitable radius as per Lemma 2.1,

$$\Phi_{B'_r}^{(s)}(x) \leq C_4 r^{d-s},$$

for all $x \in M$, where $C_4 := \max(C_H, 3^{d-s} C_3)$. This yields the estimate

$$\mathcal{J}_{B'_r} \left| U_x^{(s)} - U_{x'}^{(s)} \right| = O(r^{d-s}). \quad (12)$$

Secondly, let $y \in M$ be such that $\text{dist}(y, x') = r$, with $0 < r < \min(1, R_1/3)$. If $\text{dist}(x, x') = t < r$, then by the triangle inequality, $\text{dist}(x, y) \geq r - t$, and so

$$\left| \text{dist}(x, y)^{-s} - \text{dist}(x', y)^{-s} \right| \leq (r - t)^{-s} - r^{-s}.$$

From the binomial expansion of $(r - t)^{-s}$ we have

$$(r - t)^{-s} - r^{-s} = r^{-s} \left((1 - t/r)^{-s} - 1 \right) = r^{-s} O(t/r) = O(tr^{-s-1}).$$

We therefore have the estimate

$$\mathcal{J}_{M \setminus B'_r} \left| U_x^{(s)} - U_{x'}^{(s)} \right| = O(tr^{-s-1}). \quad (13)$$

We can equate the orders of the estimates (12) and (13) by setting $t := r^{d+1}$. This yields the overall estimate

$$\mathcal{J}_M \left| U_x^{(s)} - U_{x'}^{(s)} \right| = O(r^{d-s}) = O(t^{(d-s)/(d+1)}),$$

giving the result (11). \square

Remark. The result (11) and its proof is split into two lemmas, 2.5 and 2.6, to make the exposition easier to understand.

3 Proof of Theorem 1.1

Fix the manifold M and therefore fix d . Fix $s \in (0, d)$, and drop all superscripts (s) from the notation, where this does not cause confusion. Fix a sequence \mathcal{X} having the required properties. Fix ℓ , drop all subscripts ℓ , and examine the spherical code $X := \{x_1, \dots, x_N\}$, so that $|X| = N$. The notation of the proof also uses the abbreviations $\Delta := \Delta(N)$, $\delta := \delta(N)$.

The first observation is that

$$\begin{aligned} (E_X - E_M)U &= \mathcal{J}_X \Phi_X - \mathcal{J}_M \Phi_M \\ &= (\mathcal{J}_X \Phi_X - \mathcal{J}_X \Phi_M) + (\mathcal{J}_X \Phi_M - \mathcal{J}_M \Phi_M) \\ &= \mathcal{J}_X (\Phi_X - \Phi_M) + (\mathcal{J}_X - \mathcal{J}_M) \Phi_M. \end{aligned}$$

The first part of the proof concentrates on the convergence to 0 of the term $\mathcal{J}_X(\Phi_X - \Phi_M)$. Since

$$\mathcal{J}_X(\Phi_X - \Phi_M) = \frac{1}{N} \sum_{x \in X} (\Phi_X(x) - \Phi_M(x)) \quad (14)$$

the proof proceeds by placing a uniform bound on the net mean potential $\Phi_X(x) - \Phi_M(x)$ at $x \in X$. We express this net mean potential as a difference between Riemann-Stieltjes integrals, then integrate by parts.

Fix $x \in X$. The volume of the ball $B(x, r)$ with respect to the punctured normalized counting measure $\sigma_X^{[x]}$ is

$$\mathcal{V}_X^{[x]}(r) := \sigma_X^{[x]}(B(x, r)) = \frac{|B(x, r) \cap X| - 1}{N}.$$

Using $\mathcal{V}_M(r) := \sigma_M(B(x, r))$ to denote the volume of $B(x, r)$ with respect to the measure σ_M , and integrating by parts, yields

$$\begin{aligned} \Phi_X(x) - \Phi_M(x) &= \mathcal{J}_X^{[x]} U_x - \mathcal{J}_M U_x \\ &= \int_M U(\text{dist}(x, y)) d\sigma_X^{[x]}(y) - \int_M U(\text{dist}(x, y)) d\sigma_M(y) \\ &= \int_0^\infty r^{-s} d\mathcal{V}_X^{[x]}(r) - \int_0^\infty r^{-s} d\mathcal{V}_M(r) \\ &= \int_0^\infty sr^{-s-1} \mathcal{V}_X^{[x]}(r) dr - \int_0^\infty sr^{-s-1} \mathcal{V}_M(r) dr \\ &= \int_0^\infty sr^{-s-1} (\mathcal{V}_X^{[x]}(r) - \mathcal{V}_M(r)) dr. \end{aligned} \quad (15)$$

We now bound $|\Phi_X(x) - \Phi_M(x)|$ by placing an upper bound on each of $\mathcal{V}_X^{[x]}(r) - \mathcal{V}_M(r)$ and its negative, $\mathcal{V}_M(r) - \mathcal{V}_X^{[x]}(r)$.

Because the minimum distance between points of X is bounded below by Δ , each point of X can be placed in a ball of radius $\Delta/2$, with no two balls overlapping. Lemma 2.3 then implies that for $r < \text{diam}(M)$,

$$|B(x, r) \cap X| \leq n_M(x, r + \Delta/2, \Delta/2) \leq C_2 (r/\Delta)^d,$$

and so

$$\mathcal{V}_X^{[x]}(r) \leq C_2 \Delta^{-d} N^{-1} r^d - N^{-1}.$$

Since the normalized spherical cap discrepancy $\mathcal{D}(X)$ is bounded above by δ , it is also true that for $0 < r < \text{diam}(X)$,

$$-\delta \leq \mathcal{V}_X^{[x]}(r) - \mathcal{V}_M(r) + N^{-1} \leq \delta.$$

Let $\rho := \delta^{1/d}$. Since δN is at least $\Omega(1)$, and since X is well separated,

$$0 < \Delta < \rho < \text{diam}(M),$$

for N sufficiently large. Since the minimum distance between points of X is bounded below by Δ , $\mathcal{V}_X^{[x]}(r) = 0$ when $r < \Delta$. Since σ_M and σ_X are probability measures on M , $\mathcal{V}_M(r) = 1$ and $\mathcal{V}_X^{[x]}(r) = (N-1)/N$ when $r \geq \text{diam}(M)$.

The simple lower bound $\mathcal{V}_M(r) \geq 0$ for $0 < r \leq \rho$, and the bounds immediately above yield the following cases for the upper bound on $\mathcal{V}_X^{[x]}(r) - \mathcal{V}_M(r)$:

$$\mathcal{V}_X^{[x]}(r) - \mathcal{V}_M(r) \leq \begin{cases} 0, & r \in [0, \Delta], \\ C_2 \Delta^{-d} N^{-1} r^d - N^{-1}, & r \in (\Delta, \rho), \\ \delta - N^{-1}, & r \in [\rho, \text{diam}(M)], \\ -N^{-1}, & r \geq \text{diam}(M). \end{cases}$$

Substitution back into (15) results in the uniform upper bound

$$\begin{aligned} \Phi_X(x) - \Phi_M(x) &= \int_0^\infty s r^{-s-1} (\mathcal{V}_X^{[x]}(r) - \mathcal{V}_M(r)) dr \\ &\leq C_2 \Delta^{-d} N^{-1} s \int_\Delta^\rho r^{d-s-1} dr \\ &\quad + \delta \int_\rho^{\text{diam}(M)} s r^{-s-1} dr - N^{-1} \int_\Delta^\infty s r^{-s-1} dr \\ &= C_2 \Delta^{-d} N^{-1} \frac{s}{d-s} (\rho^{d-s} - \Delta^{d-s}) \\ &\quad + \delta (\rho^{-s} - \text{diam}(M)^{-s}) - N^{-1} \Delta^{-s}. \end{aligned}$$

Noting that $\Delta^d N = O(1)$, substituting in the value for ρ , and noting that δN is at least $\Omega(1)$, results in the bound

$$\Phi_X(x) - \Phi_M(x) \leq O(\rho^{d-s}) + O(\delta \rho^{-s}) = O(\delta^{1-s/d}). \quad (16)$$

Arguments similar to those for the upper bound on $\mathcal{V}_X^{[x]}(r) - \mathcal{V}_M(r)$ result in the cases

$$\mathcal{V}_M(r) - \mathcal{V}_X^{[x]}(r) \leq \begin{cases} C_H r^d, & r \in [0, \rho], \\ \delta + N^{-1}, & r \in (\rho, \text{diam}(M)), \\ N^{-1}, & r \geq \text{diam}(M). \end{cases}$$

Substitution back into (15) results in the uniform upper bound

$$\begin{aligned} \Phi_M(x) - \Phi_X(x) &= \int_0^\infty s r^{-s-1} (\mathcal{V}_M(r) - \mathcal{V}_X^{[x]}(r)) dr \\ &\leq C_H s \int_0^\rho r^{d-s-1} dr - \delta \int_\rho^{\text{diam}(M)} s r^{-s-1} dr + N^{-1} \int_\rho^\infty s r^{-s-1} dr \\ &= C_H \frac{s}{d-s} \rho^{d-s} + \delta (\text{diam}(M)^{-s} - \rho^{-s}) + N^{-1} \rho^{-s}. \end{aligned}$$

Similarly to the argument for the upper bound on $\Phi_X(x) - \Phi_M(x)$, this gives the bound

$$\Phi_M(x) - \Phi_X(x) \leq O(\rho^{d-s}) + O(N^{-1} \rho^{-s}) = O(\delta^{1-s/d}). \quad (17)$$

When the upper bounds (16) and (17) are combined, this results in the overall order estimate

$$|\Phi_X(x) - \Phi_M(x)| = O(\delta^{1-s/d}).$$

Therefore, recalling the sum (14), this shows that

$$\mathcal{J}_X(\Phi_X - \Phi_M) = O(\delta^{1-s/d}). \quad (18)$$

We now treat the convergence of the term $(\mathcal{J}_X - \mathcal{J}_M)\Phi_M$ to 0 as $N \rightarrow \infty$.

Since Φ_M is continuous on M as per Lemma 2.5, and since the sequence \mathcal{X} is asymptotically equidistributed, with each measure σ_X being a probability measure on M , by Blümlinger's Theorem 2 [3, p. 181], the term $(\mathcal{J}_X - \mathcal{J}_M)\Phi_M$ converges to 0 as $N \rightarrow \infty$. To obtain a rate of convergence for this term, we use Blümlinger's Theorem 1 [3, p. 180] along with Lemma 2.6.

We adopt Blümlinger's notation, and set $f := \Phi_M$, $\lambda := \lambda_M$, $\mu := \lambda$, $\nu := \lambda(M)\sigma_X$. We also adjust Blümlinger's estimate to take into account that in our case $\lambda(M)$ is not necessarily 1. The estimate in this case is

$$|\nu(f) - \lambda(f)| \leq T_1(r) + T_2(r) + T_3(r), \quad (19)$$

where

$$\begin{aligned} T_1(r) &:= \|f - f_r\| \|\nu\|, \\ T_2(r) &:= \|f\| (\|\nu\| + \|\lambda\|) K(r), \\ T_3(r) &:= \frac{\|f\|}{\lambda_0(r)} \int_M |\nu(B(x, r)) - \lambda(B(x, r))| d\lambda(x). \end{aligned}$$

The norm used here is $\|\cdot\|_\infty$, the norm on $C(M)$. Therefore $\|\nu\| = \|\lambda\| = \lambda(M)$.

We now estimate the order of each term with respect to r and the discrepancy bound δ . For $T_1(r)$ we find the extrema of f and f_r on M . From Blümlinger's definition of f_r , [3, p. 179] we see that f_r is the mean on $B(x, r)$ of f with respect to λ . It therefore holds that

$$\min_{x \in B(x, r)} f(x) \leq f_r(x) \leq \max_{x \in B(x, r)} f(x).$$

Recalling that $f = \Phi_M$, and applying the estimate (11) from Lemma 2.6, we obtain

$$\|f - f_r\| = O(r^{(d-s)/(d+1)})$$

for r sufficiently small. Therefore

$$T_1(r) = O(r^{(d-s)/(d+1)}). \quad (20)$$

For $T_2(r)$, Blümlinger's estimate 4 as per Lemma 1.2 yields $T_2(r) = O(r^2)$.

For $T_3(r)$, first note that

$$\frac{\|f\|}{\lambda_0(r)} = O(r^{-d}).$$

Since

$$|v(B(x, r)) - \lambda(B(x, r))| \leq \delta,$$

this yields

$$T_3(r) = O(\delta r^{-d}). \quad (21)$$

To equate the orders of the estimates (20) and (21) for $T_1(r)$ and $T_3(r)$, we set $r = \delta^{(d+1)/(d^2+2d-s)}$. This results in an overall estimate of

$$(\mathcal{I}_X - \mathcal{I}_M)\Phi_M = \frac{1}{\lambda(M)}(v(f) - \lambda(f)) = O(\delta^{(d-s)/(d^2+2d-s)}). \quad (22)$$

The estimates (18) and (22) combine to yield the estimate (3). \square

4 Discussion

Theorem 1.1 demonstrates the convergence of the normalized Riesz s -energy of a well separated, equidistributed sequence of M -codes on a compact connected d -dimensional Riemannian manifold M to the energy given by the double integral of the normalized volume measure on M , in the case where $0 < s < d$. The estimated rate of convergence given by the theorem is much slower than the corresponding rate of $\delta^{1-s/d}$ on the sphere [19].

The proof of Theorem 1.1 relies on the estimate (19) from Blümlinger's Theorem 1 [3]. This, to some extent, resembles a Koksma-Hlawka-type inequality, in that it contains three terms, each of which separate the dependence on the function and the dependence the measure into different factors. One key difference between the estimate (19) and a Koksma-Hlawka-type inequality is that the term T_3 has $\lambda_0(r)$ in the denominator. This makes it difficult to apply this estimate to the case of arbitrarily small positive r .

If the manifold M actually had a Koksma-Hlawka-type inequality for the ball discrepancy δ , with a function space F_M containing the function Φ_M , the estimate

$$|(\mathcal{I}_X - \mathcal{I}_M)\Phi_M| \leq \delta V(\Phi_M)$$

would hold for some appropriate functional V on the space F_M . Unfortunately, not much is known about Koksma-Hlawka type inequalities for geodesic balls on compact connected Riemannian manifolds, with the exception of the sphere \mathbb{S}^d [6, Section 3.2, p. 490] [7, Proposition 20].

The papers by Brandolini et al. [4, 5] examine Koksma-Hlawka type inequalities on compact Riemannian manifolds. The main results of those two papers concern discrepancies which are not in general the same as the geodesic ball discrepancy, but they do suggest directions for further research.

Further research could address the following questions.

1. For a compact connected Riemannian manifold M , for what linear spaces F_M does a Koksma-Hlawka type inequality

$$|(\mathcal{I}_X - \mathcal{I}_M)f| \leq \mathcal{D}(X) V(f) \quad (23)$$

hold for all $f \in F_M$, where the relevant discrepancy in the inequality is the geodesic ball discrepancy?

2. What is the appropriate functional V in (23)? Is V a norm or a semi-norm on the function space F_M ?
3. For which compact connected Riemannian manifolds M does the Koksma-Hlawka function space F_M contain the mean potential function Φ_M ?

Finally, no mention has yet been made of constructions for, or even the existence of, well separated, admissible sequences on compact connected Riemannian manifolds. The case of the unit sphere \mathbb{S}^d has been well studied [19] and a number of constructions are known, including one that uses a partition of the sphere into regions of equal volume and bounded diameter [18].

Damelin et al. have studied the discrepancy and energy of finite sets contained within measurable subsets of Hausdorff dimension d embedded in a higher dimensional Euclidean space, where the energy and discrepancy are both defined via an admissible kernel [9]. One of their key results is to express the discrepancy of a finite set with respect to an equilibrium measure as the square root of the difference between the energy of the finite set and the energy of the equilibrium measure [9, Corollary 10]. They have also studied the special case where both the measurable subset and the kernel are invariant under the action of a group [9, Section 4.3]. This case includes compact homogeneous manifolds [10].

The methods of Damelin et al. might be used to prove the equidistribution of a sequence of M -codes \mathcal{X}^* , where each code X_ℓ^* has the minimum Riesz s -energy of all codes of cardinality $|X_\ell^*|$. Much care must be taken: although their definition of an admissible kernel includes the Riesz s -kernels as defined in this paper [9, Section 2.1], their definitions and results are framed in terms of sets embedded in Euclidean space, their definition of discrepancy is given in terms of a norm depending on the kernel [9, (8)], the measure used in their Corollary 10 is the equilibrium measure, not the uniform measure, and their definition of energy includes the diagonal terms excluded in this paper, so that the energy of the Riesz s -kernel on a finite set is infinite [9, (5) and Section 3].

Brandolini et al. [4, p. 2] give an example where the existence of a partition of the manifold M into N regions, each with volume N^{-1} and diameter at most $cN^{-1/d}$, yields an M -code X obtained by selecting one point from each region, and this gives a bound on the quadrature error of the code X with respect to bounded functions on the manifold M . Such a partition might be constructed by adapting the modified Feige-Schechtman partition algorithm for the unit sphere [11] [18, 3.11.4, pp. 145-148]. Care must be taken to adapt the algorithm, in particular to choose an appropriate radius for the initial saturated packing of the manifold M by balls of a fixed radius. Also, it would need to be proven that the adapted algorithm works for all compact connected Riemannian manifolds and all cardinalities N .

A recent paper by Ortega-Cerdà and Pridhnani [20] treats sequences of Fekete point sets on some types of smooth compact connected Riemannian manifolds M , showing that such sequences are uniformly separated [20, Theorem 9] and asymptotically equidistributed [20, Theorem 11]. Uniform separation [20, p. 2106] is defined in terms of the orthonormal basis for $L^2(M)$ consisting of eigenfunctions of the Laplacian operator on M , as opposed to the purely geometric concept of well-separation used in this paper. Fekete point sets are defined by maximizing the determinant of a Vandermonde matrix defined by the values of each of the basis eigenfunctions at each of the points [20, Definition 8]. These point sets are therefore determined numerically by using optimization methods rather than by construction.

Clearly, further research is needed to address the construction on compact connected Riemannian manifolds of sequences of point sets that are both equidistributed and well-separated.

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